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High pressure experiments and simulations in cocurrent bubble columns

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Abstract

Bubble column is a multiphase reactor in which gas is passes through the liquid in two phase flow. When liquid is stationary the operation is called as batch mode and co-current when both gas and liquid are moving in the same direction. The gas hold-up increases with increase in pressure for both batch & co-current column. This increment in gas holdup is very sharp initially, but soon it becomes insignificant. The increase in liquid velocity decreases the gas hold-up at all pressures. As we increase the pressure, the effect of liquid velocity is less. Three dimensional Euler-Euler two-phase fluid model has been used to simulate two-phase up-flow in bubble column (15cm diameter) using ANSYS 12.1. These experiments and simulations were operated over a range of superficial gas velocities (1 to10 cm/s) at ambient conditions as well as high pressures. The liquid velocity range was 0 to 16 cm/s. The turbulence in the liquid phase has been modeled using the standard k-ε model. The interactions between the two phases are described through Schiller Neumann drag coefficient formulation. The objectives are to find the effect of pressure and liquid velocity over gas holdup and to validate the CFD simulations with experimental data. Quantitatively good agreements are obtained between experimental data for hold-up and simulation values. Radial gas holdup profiles and axial liquid velocity profiles were also obtained for the simulation.

Keywords: Co-current flow; gas hold-up; high pressure;three dimensional simulation

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1. Introduction

Bubble columns are used in the methanol synthesis, resid hydro-treating, Fischer-Tropsch synthesis and benzene hydrogenation at high pressures [1]. The gas hold-up increases considerably as the pressure is increased for both homogeneous and heterogeneous regimes [2, 3]. Increase in pressure delays the transition from homogeneous to heterogeneous regime by reducing the probability of propagation of instabilities [4]. It also enhances the breakup of the large bubbles due to decreased bubble stability as shown by Letzel et al. using the Kelvin–Helmoltz stability analysis [3]. Because of these two reasons, the gas hold-up increases with increase in pressure. Fan et al have shown that with an increase in pressure the rise velocity of bubbles in liquids and liquid-solid suspensions decreases, which also attributes for higher gas hold-up [5]. Li et al have shown that increase in pressure reduces the bubble size formed at the sparger, thus increasing the hold-up [6]. All of them have studied the batch operation mode only. Behkish in his experiments on N_2 and He in Isopar-M has shown that the increase of gas hold-up with pressure is mainly due to holdup of small bubbles, whereas hold-up of large bubbles remains constant [7]. In addition, he reports that the gas holdup also increases with increasing superficial gas velocity and temperature [7]. Ishiyama et al. found that there was no effect of pressure on gas holdup when a single nozzle of 4.0 mm was used, but when a single nozzle of 1.0 mm was used, the pressure effect was observed [8].

Computational fluid dynamics (CFD) has gained wide attention for bubble column, because of its ability to predict the fluid hydrodynamics properly. Two main approaches are generally used while modeling gas-liquid flow in bubble columns: Euler-Euler (E-E) [9] and Euler-Lagrange (E-L) [10]. The E-E approach (the two-fluid model) considers the gas and liquid phases as two interpenetrating fluids in a eulerian framework. The phases interact through the inter-phase transfer terms [11]. On the contrary, in the E-L approach the liquid phase is treated as a continuum; and in the gas phase each bubble is tracked separately. It's easy to introduce coalescence, break-up and collisions in the E-L model, but it's computationally very expensive due to tracking of each bubble separately. Additionally, E-E simulations are applicable to a wider range of volume fractions, while E-L is restricted to low particle volume fractions as the fraction of volume taken by the particles is not included in the continuous phase calculation. Furthermore, the use of high order discretization schemes with the E-E approach solve the problem of the higher numerical diffusion obtained in comparison with the E-L approach, as found by Sokolichin et al. [12].

In this present work E-E approach is adapted. All the simulations are done using ANSYS 12.1. The aim of this work is to study the effect of pressure and liquid velocity over gas hold-up in a co-current bubble column and also to validate the experimental gas hold-up with simulation values.

2. Experimental Set-up

The column is 2.72 m long and made of stainless steel (SS-304). Its inner diameter is 15.4 cm. Thickness of the material is 5 mm. 5 ports have been welded to it at different locations for measuring the pressure through differential pressure transducers. These are piezoelectric sensors supplied by the Honeywell International, USA (ST 3000 Smart Pressure Transmitter). A pressure release valve has been installed in the top section of the column. The whole set-up has been tested to withstand a pressure of 13 bars. The diameter of tank is 96 cm and thickness of the material is 5 mm. Total height of tank is 115 cm. Volume of tank is 850 liters. The outlet of the column is maintained at the operating pressure using the back pressure regulator. In the separator the gas and liquid phase separate out and gas phase is discharged to ambient with the help of a pressure release valve. The volume of the separator is 175 liter. The liquid velocity has been varied from 0 to 12.26 cm/s. The gas velocity range is 0 to 16.28 cm/s. Line diagram of the setup has been shown in Fig. 1.

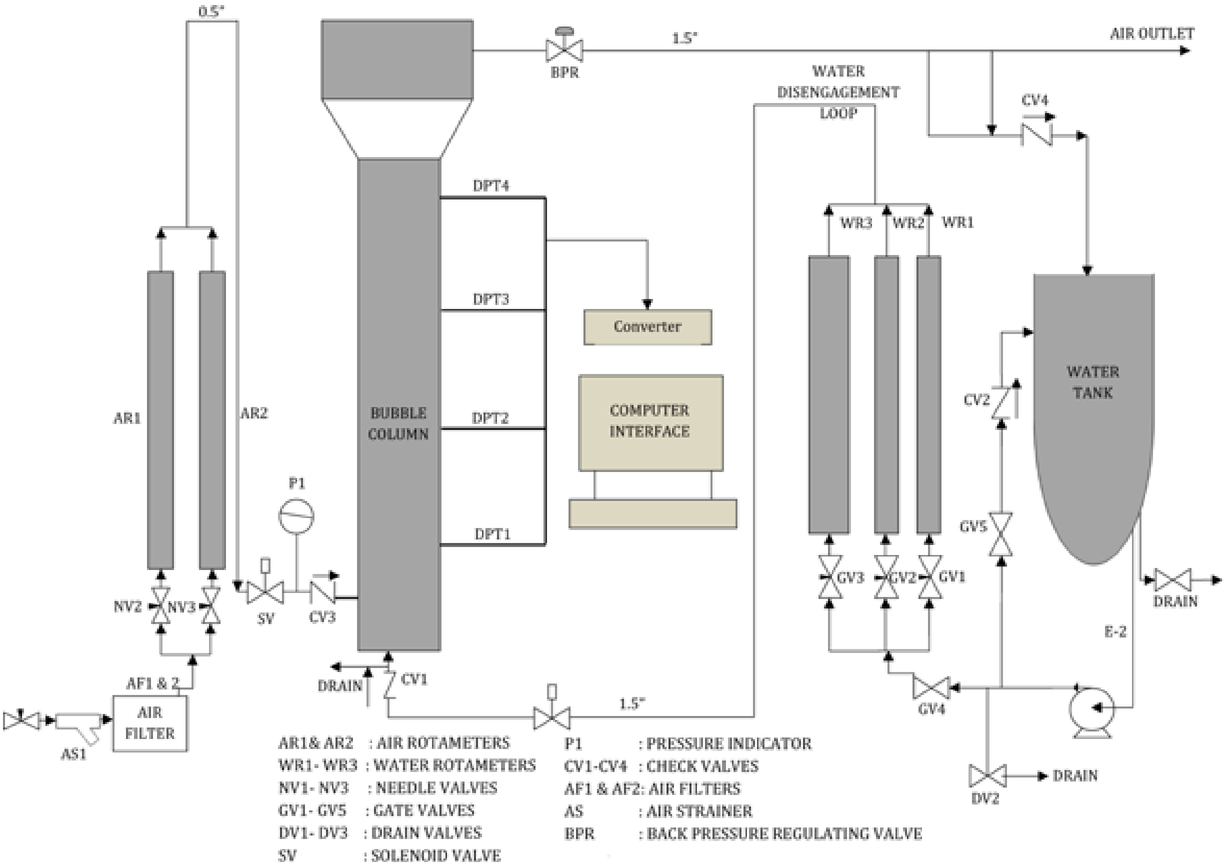

Fig. 1. Line Diagram of the high pressure experimental set-up

Compressed atmospheric air is used as gas phase. It is passed through a strainer to separate large dust particles. Two air filters, of mesh size 40 μm and 1 μm are connected in series, to prevent any solid particles and liquid droplets or oil mist to enter the column which may act as contaminant and may influence the results. Tap water is used as liquid phase. Spider sparger with orifice diameter 1 mm and 120 holes has been used to pass the gas at the inlet of the column. For measuring the liquid velocity, Electromagnetic Flow meter (Krohne Marshall, Model no AQUAMAG) is used. The air flow rate has been measured using the rotameter (Eureka model no PG-1 & PG-2). Differential Pressure transducers (DPTs) have been used to measure the pressure difference between two ports of the column. Data Acquisition card (DAQ card), PCI-6024E (National Instruments) has been installed in an Intel PC for collecting the data from the DPT's. For each run, the data has been acquired for 200 sec with 50 Hz frequency.

Tang and Heindel have developed equation (1) to calculate the average gas hold-up [13].

$$\varepsilon = 1 - \frac{\Delta P}{\Delta P_{0,U_l}} \quad (1)$$

where ΔP = is the pressure difference between the lower and higher ends of column section and $\Delta P_{0,Ul}$ is the corresponding static pressure difference when no gas is flowing in the column, keeping all other conditions as same. Equation (1) neglects the effect of wall shear stress and liquid acceleration due to void changes that may influence gas holdup in cocurrent bubble columns [14, 15]. In our case the effect of wall shear stress is negligible, since the wall shear stress is significant only after U_l> 40 cm/s for air water system [16]. Hence, we have applied equation (1) for calculating the gas holdup values.

3. Results & Discussion

3.1. Effect of liquid velocity at high pressure

At atmospheric conditions, Shah et al. [17] studied the effect of liquid velocity in a downward flow bubble column. Tang and Heindel [18] studied the effect of sparger orientation in cocurrent and batch flow and observed a decrease in holdup with increasing liquid velocity. In cocurrent flow, the liquid velocity reduces the relative velocity between the liquid and gas and hence, the bubble- induced turbulence intensity. Hills [14] reported a decrease in gas holdup with an increase in liquid velocity (0 – 2.7 m/s). Fujie et al. [19] and Friedel et al. [20] also reported a decrease in gas holdup with an increase in liquid velocity in down flow bubble columns of 45 cm and 15 cm internal diameter, respectively.

In the present work, the effect of liquid velocity has been studied at pressures 1, 3 , 5 and 7 bar. The range of liquid velocity is from 0 to 16 cm/s. It was found that the increase in liquid velocity decreases the gas hold-up even at high pressures. It consistently decreases with increase in liquid velocity. As the liquid phase momentum is increased, the momentum transferred to the gas phase increases. It reduces the residence time of a bubble, hence the overall hold-up. This has been shown in Fig 2 and 3.

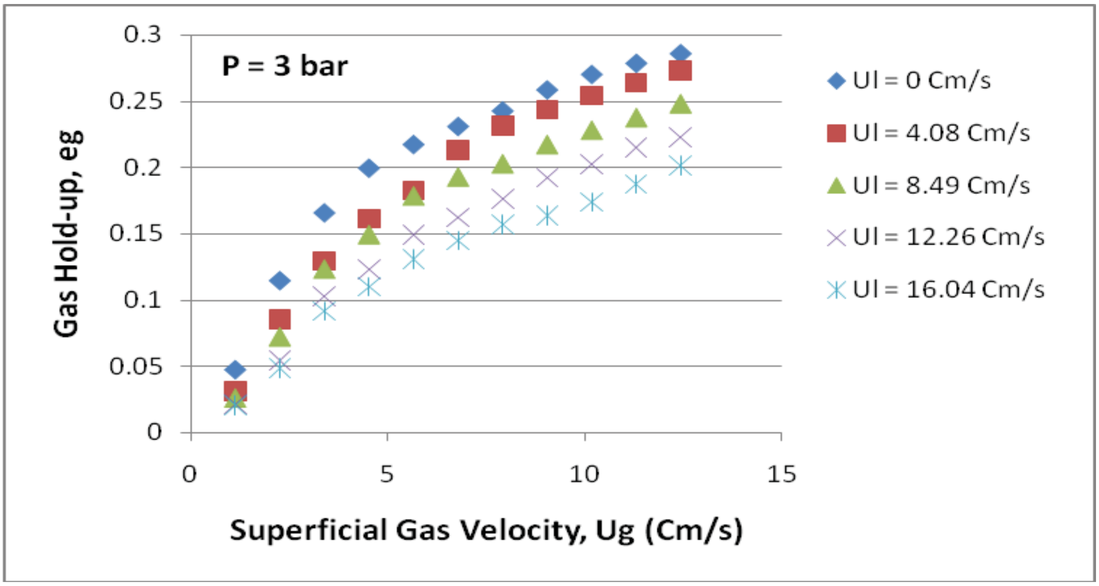

Fig. 2. Effect of Liquid Velocity over Gas Hold-up at 3 bar

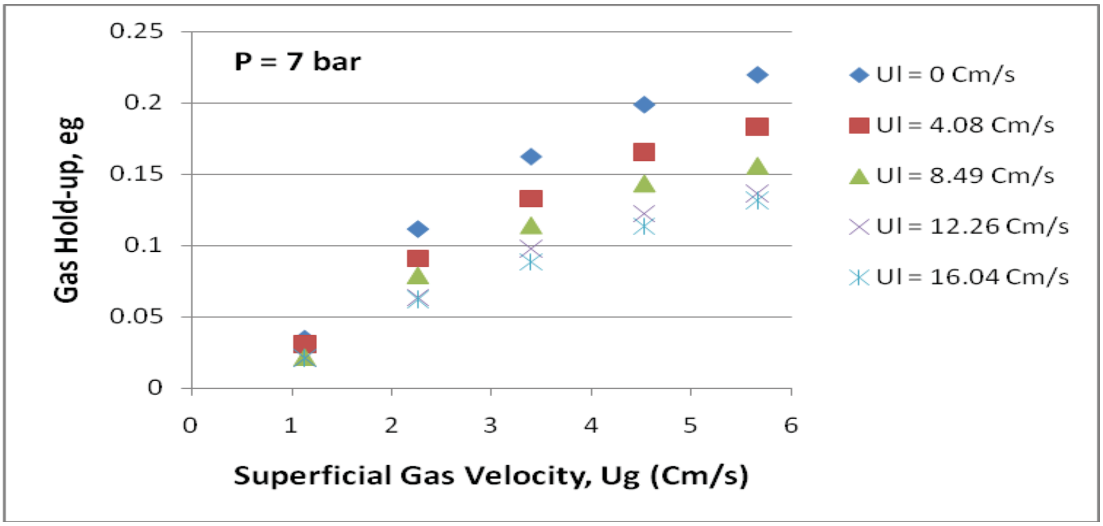

Fig. 3. Effect of Liquid Velocity over Gas Hold-up at 7 bar

Table 1. Effect of Liquid velocity over gas Hold-up at 1 bar

Superficial Gas Velocity (U_g) ↓	Gas Hold-up (ε_g)				
U_l →	0.000	4.080	8.490	12.260	16.040
1.13	0.023	0.018	0.015	0.014	0.015
2.26	0.038	0.030	0.025	0.024	0.023
3.40	0.052	0.043	0.034	0.032	0.030
3.96	0.058	0.048	0.040	0.037	0.033
4.53	0.067	0.055	0.045	0.041	0.038
5.10	0.075	0.062	0.050	0.046	0.042
5.66	0.082	0.067	0.055	0.049	0.046
6.23	0.090	0.073	0.062	0.053	0.048
6.79	0.100	0.081	0.067	0.060	0.053
7.93	0.120	0.096	0.081	0.070	0.063
9.06	0.138	0.114	0.094	0.080	0.072
10.19	0.161	0.130	0.109	0.091	0.080
11.32	0.175	0.148	0.119	0.104	0.090
12.46	0.194	0.159	0.135	0.112	0.101
13.59	0.208	0.176	0.145	0.126	0.109
14.72	0.219	0.186	0.158	0.135	0.119
16.28	0.233	0.200	0.172	0.149	0.131

The value of gas hold-up at different liquid and gas velocity has been tabulated in Table 1. The hold-up continues to increase with respect to superficial gas velocity as shown in the Table 1.

3.2. Effect of Pressure over gas hold-up

The holdup in general is seen to increase with pressure regardless of the composition of the liquid [21, 22]. The increased pressure leads to smaller bubble sizes and consequently higher holdups and high interfacial areas. An increase in viscosity of the liquid phase decreases the amount of large bubbles in the churn turbulent flow regime; the flow becomes less compressible and unaffected by an increase in pressure [23]. For liquids with low viscosity, both superficial gas velocity and pressure play an equally important role and affect the bubble size distribution. Kang et al using chaos analysis concluded that at high pressures a homogenous bubbly regime can be maintained at higher superficial gas velocities [24, 25]. Effect of pressure for different superficial liquid velocities has been shown in Figure 4-6.

An increase in pressure increases the hold-up for a constant liquid velocity. As we increase the liquid velocity, the difference between hold-up at 1 and 3 bar decreases. It was observed that when we increase the pressure from atmospheric conditions, the holdup increases sharply. Afterwards this increment in the holdup wrt pressure is slow. So, increase in the pressure increases the holdup but with a tapering effect. The first increment of pressure from 1 atm shows a sudden step change or a sharp increment (i.e a quantum jump) in the holdup. However, subsequent increases in pressure show a relatively much smaller increment in the holdup.

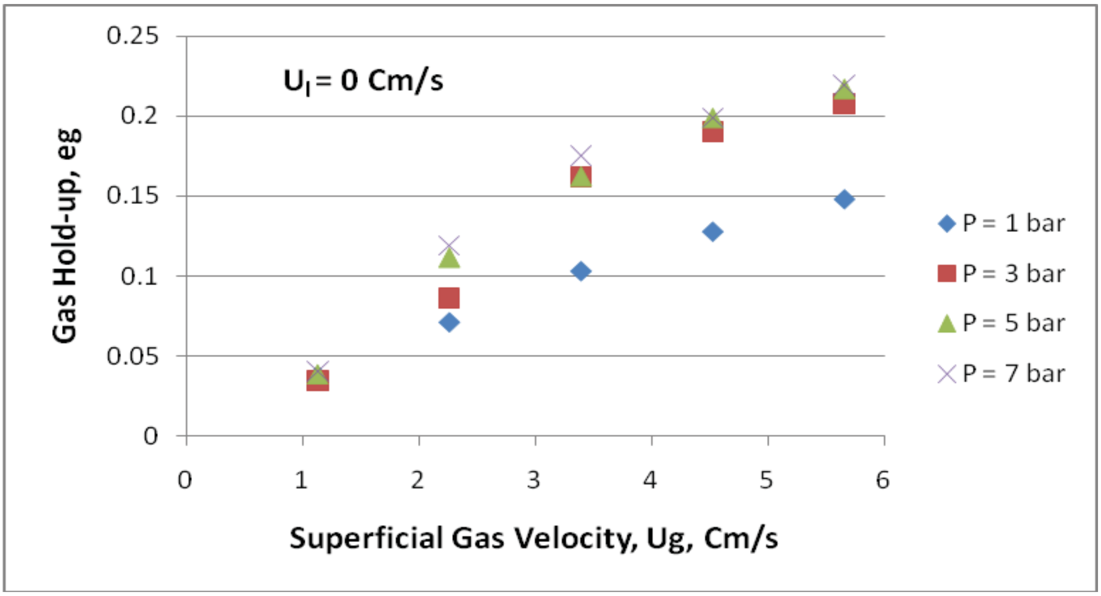

Fig. 4. Effect of Pressure over gas hold-up at $U_l = 0$ cm/s

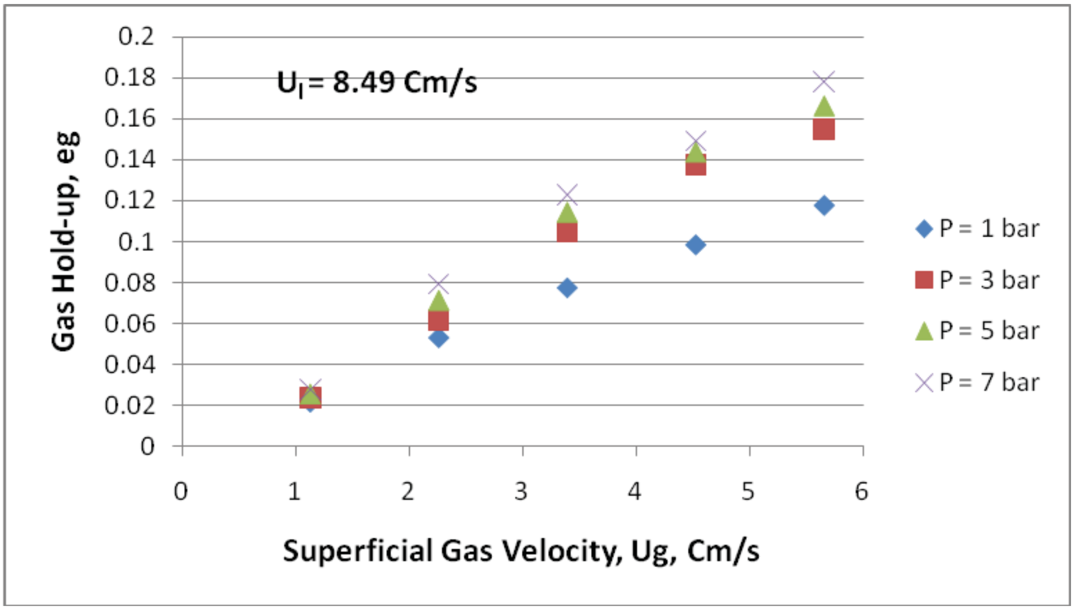

Fig. 5. Effect of Pressure over gas hold-up at U_l = 8.49 cm/s

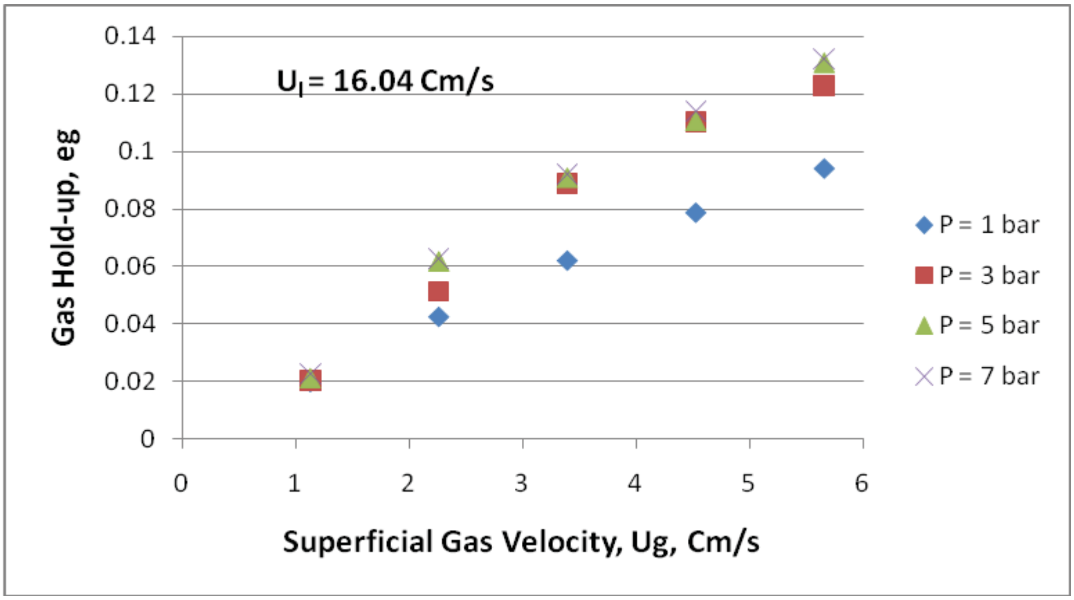

Fig. 6. Effect of Pressure over gas hold-up at U_l = 16.04 cm/s

4. Simulation

4.1. Euler-Euler model

Here continuity and momentum equations for each phase need to be solved. The continuity equation is given by

$$\sum_{\alpha=1}^{N_p} \varepsilon_\alpha = 1 \tag{2}$$

$$\frac{\partial}{\partial t}\varepsilon_\alpha \rho_\alpha + \nabla.\left(\varepsilon_\alpha\left(\rho_\alpha U_\alpha\right)\right) = 0 \tag{3}$$

The momentum equation is given by

$$\frac{\partial}{\partial t}\varepsilon_\alpha \rho_\alpha U_\alpha + \nabla.\left(\varepsilon_\alpha\left(\rho_\alpha U_\alpha U_\alpha - \mu_\alpha\left(\nabla U_\alpha + (\nabla U_\alpha)^T\right)\right)\right) = \varepsilon_\alpha\left(\rho g - \nabla p_\alpha\right) + \sum_{\beta=1}^{N_p} c_{\alpha\beta}^{(d)}\left(U_\beta - U_\alpha\right) \tag{4}$$

4.2. Turbulence models

The equation for turbulent kinetic energy (k) is described as

$$\frac{\partial}{\partial t}\left(\rho_\alpha \varepsilon_\alpha k\right) + \nabla\left(\rho_\alpha \varepsilon_\alpha \overline{v}_\beta k\right) = -\nabla\left(\frac{\mu_t}{\sigma_k}\nabla k\right) + \varepsilon_\alpha\left(G - \rho_\alpha \varepsilon\right) \tag{5}$$

while the equation for dissipation rate (ε) is

$$\frac{\partial}{\partial t}\left(\rho_\alpha \varepsilon_\alpha \varepsilon\right) + \nabla\left(\rho_\alpha \varepsilon_\alpha \overline{v}_\beta \varepsilon\right) = -\nabla\left(\frac{\mu_t}{\sigma_\varepsilon}\nabla \varepsilon\right) + \varepsilon_\alpha\left(C_1 G - C_2 \rho_\alpha \varepsilon\right) \tag{6}$$

The term G in the in both turbulent kinetic energy (k) and turbulent dissipation rate (ε) equations is defined as

$$G = \tau_\alpha : \nabla \overline{v}_\alpha \tag{7}$$

The turbulent viscosity, μ_t is calculated as:

$$\mu_t = \rho C_\mu \frac{k^2}{\varepsilon} \tag{8}$$

The model constants for Standard k-ε turbulence model are $C_\mu = 0.09$; $\sigma_k = 1$; $\sigma_\varepsilon = 1.3$; $C_1 = 1.44$; $C_2 = 1.92$.

4.3. Simulation Methodology

A three dimensional grid has been made in GAMBIT 2.3 having 2,86,000 hexagonal cells. The simulation domain starts at the sparger and ends at the top of the column. The terminal rise velocity has been calculated using correlation given by Mandelson [26]

$$V_t = \sqrt{\frac{\sigma}{r_b * \rho_l} + g * r_b} \tag{9}$$

Here σ is the surface tension of liquid phase, r_b is the radius of the bubble, ρ_l is the density of the liquid phase and g is acceleration due to gravity.

Inlet variable values were specified based on the mode of flow - batch or co-current. Gas phase inlet velocity has been specified as the terminal rise velocity for batch column. No slip condition was applied at all the walls. Outlet has been defined as pressure outlet and inlet as velocity inlet. For all simulations, a time step was of 0.01 seconds was used with total flow time of 100 seconds. SIMPLEC technique has been used for pressure-velocity coupling [27]. The under relaxation values for pressure and momentum equation were set to 0.6 and 0.4 respectively. First order upwind scheme has been used for discretization of differential equations. For co-current flow of both the phases, the same technique applied for batch case has been applied. However in this simulation, at t= 0 sec, the column was assumed to be empty, and both the phases were allowed to enter the column. Schiller-Neumann [28] drag force model has been used for present work.

4.4. Results and Discussion

The experimental and simulation values have been compared in Figure 7 for U_l = 4.08 cm/s.

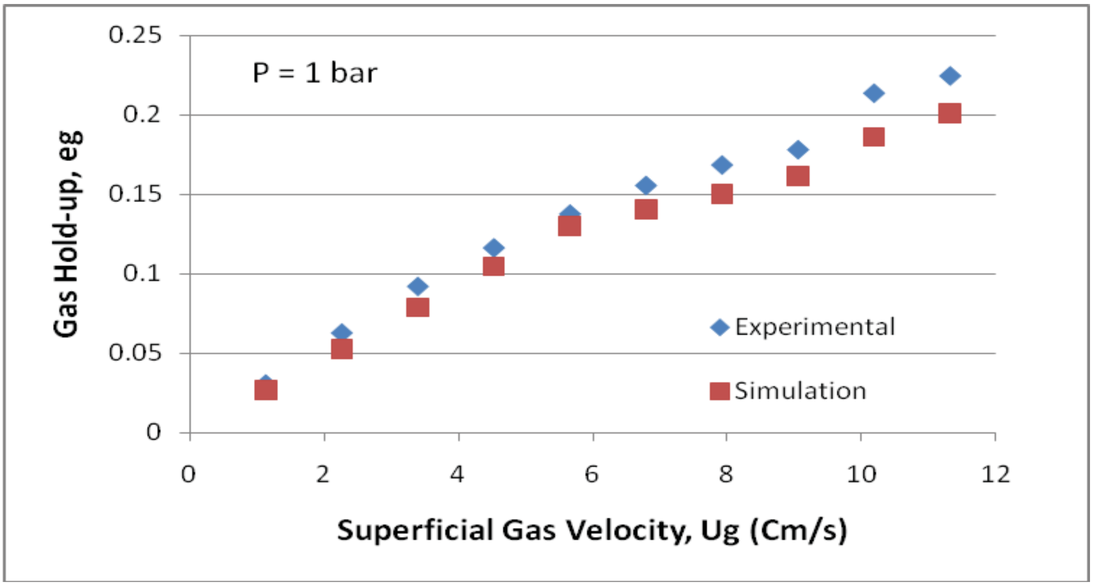

Fig. 7. Comparision of experimental and simulation gas hold-up values

It is observed from Figure 7 that the difference between experimental and simulation values are less for Ug < 6 cm/s. Afterwards the deviation increases. This is due to the assumption of constant bubble size of 5 mm. This assumption is true only for low gas velocities. For high gas velocities different sizes of bubbles exist due to coalescence and breakup. So, Population Balance Module needs to be incorporated.

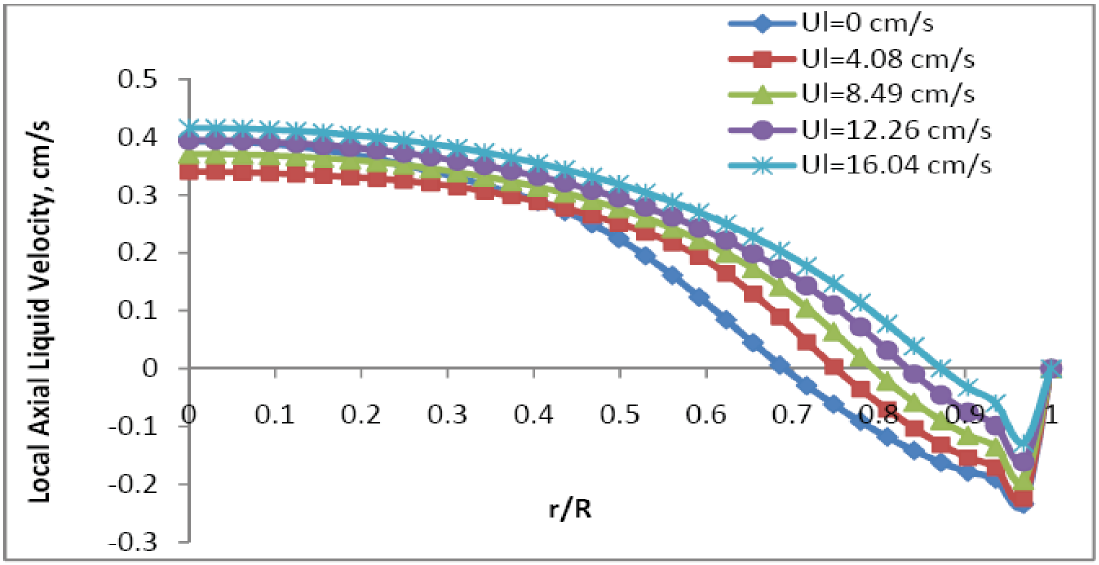

Fig. 8. Radial distribution of axial liquid velocity profiles for superficial gas velocity Ug=4.53 cm/s

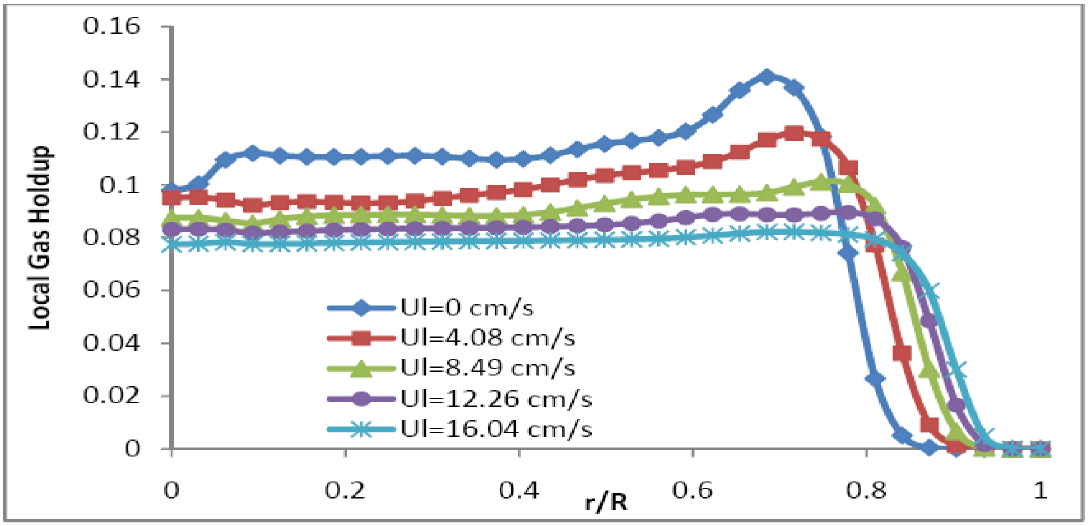

Fig. 9. Radial distribution of Gas Holdup profiles for superficial gas velocity Ug=4.53 cm/s

In the axial liquid velocity profile (Fig 8), a cross over point is observed where the axial velocity becomes zero. As the liquid velocity increases, this point shifts towards the wall of the column which results in decrease in liquid recirculation. Due to high momentum of liquid velocity, gas phase creates less circulation in the column. In the gas holdup profile, average gas holdup decreases with increasing liquid velocity. High velocity of the liquid phase reduces the residence time of bubbles in the reactor, which results in decreasing the gas holdup.

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